4-Ethyltoluene 622-96-8 | DTXSID9029194

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Model Performance	
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Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 3.95 days

Global applicability domain: Inside

Local applicability domain index: 8.72e-01

Confidence level: 8.31e-01

Nearest Neighbors from the Training Set

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4-Ethyltoluene Measured: 24.3 Predicted: 3.95 Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: 40.7 Predicted: 4.08

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1,3-Dimethyl-5-ethylbenzene

Measured: 4.93 Predicted: 3.64

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Propylbenzene Measured: 24.3 Predicted: 4.02 Image not found

1,3-Diethylbenzene Measured: 88.3 Predicted: 5.36